Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.85 days

Global applicability domain: Inside

Local applicability domain index: 7.96e-01

Confidence level: 8.18e-01

Nearest Neighbors from the Training Set

Image not found
1,2,3,5-Tetramethylbenzene
Measured: 12.5
Predicted: 3.31

Image not found
1,3,5-Trimethylbenzene
Measured: 12.5
Predicted: 3.63

Image not found
1,2,3,4-Tetramethylbenzene
Measured: 24.3
Predicted: 3.95

Image not found
para-Xylene
Measured: 157
Predicted: 5.33

Image not found
Methylcyclohexane
Measured: 24.3
Predicted: 4.12